

Analysis of stochastic time series in N dimensions in the presence of strong measurement noise

B. Lehle¹

¹bernd@vflow.de, vFlow Engineering GmbH, Pforzheimer Strasse 348, D-70499 Stuttgart, Germany

An extension and generalization of a recently presented approach for the analysis of Langevin-type stochastic processes in the presence of strong measurement noise is presented. For a stochastic process in N dimensions which is superimposed with strong, exponentially correlated, Gaussian distributed, measurement noise it is possible to extract the strength and the correlation functions of the noise as well as polynomial approximations of the drift and diffusion functions of the underlying process.

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I. INTRODUCTION

In the last years there has been significant progress in the analysis and characterization of the dynamics of processes underlying the time series of complex dynamical systems [1–4]. If the temporal evolution of a quantity $\mathbf{X}(t)$ can be described by a Langevin equation, it is possible to extract drift and diffusion functions of the underlying stochastic process from a given timeseries. This can be done because the moments of the conditional probability densities of $\mathbf{X}(t+\tau)|_{\mathbf{X}(t)=\mathbf{x}}$ can be related to these functions.

Since this approach was introduced [5–9] it has been successfully carried out in a broad range of fields. For example for data from financial markets [10], traffic flow [11], chaotic electrical circuits [12, 13], human heart beat [14], climate indices [15, 16], turbulent fluid dynamics [17], and for electroencephalographic data from epilepsy patients [18, 19].

Real-world data, however, also gives rise to some problems. One of them is, that experimental data is only given with a finite sampling rate. So methods had to be proposed to deal with the effects arising from this fact [20–24]. Another problem is the virtually unavoidable measurement noise [3, 24–26]. In the presence of measurement noise $\mathbf{Y}(t)$ the values of $\mathbf{X}(t)$ or any of its probability densities are no longer accessible, but only $\mathbf{X}^*(t) = \mathbf{X}(t) + \mathbf{Y}(t)$ and its density distributions.

Recently an approach has been presented which allows the estimation of drift and diffusion functions in the presence of strong, delta-correlated, Gaussian noise [27, 28]. Starting with initial estimates for the noise strength and the drift and diffusion functions a functional of these unknowns is iteratively minimized. An alternative approach, which is able to deal also with strong, exponentially correlated, Gaussian noise, has been presented in [29].

The aim of this paper is the formulation of this later approach in N dimensions and also its generalization. The basic idea stays the same. Instead of looking at the conditional moments in the first place, the joint probability density $\rho(\mathbf{x}, \mathbf{x}', \tau)$ of pairs $(\mathbf{X}(t), \mathbf{X}(t+\tau))$ is looked at. If the measurement noise is independent of $\mathbf{X}(t)$, then $(\mathbf{X}(t), \mathbf{X}(t+\tau))$ and $(\mathbf{Y}(t), \mathbf{Y}(t+\tau))$ are independent random variables. Hence the joint probability density $\rho^*(\mathbf{x}, \mathbf{x}', \tau)$ of their sum $(\mathbf{X}^*(t), \mathbf{X}^*(t+\tau))$ is given by the convolution of ρ and ρ_Y , where $\rho_Y(\mathbf{x}, \mathbf{x}', \tau)$ is the joint probability density of $(\mathbf{Y}(t), \mathbf{Y}(t+\tau))$.

The noise is assumed to be Gaussian and the Gauss function has some special algebraic properties. This allows to express the moments of ρ^* in terms of the moments of ρ and of the noise parameters. The obtained relations can then be used to extract the noise parameters. Furthermore, by the use of integral transforms (the Fourier transform used in [29] is a special case hereof), it is possible to extract polynomial approximations of the drift and diffusion functions using purely algebraic relations between quantities that can be calculated directly from a given, noisy time series.

This paper is organized as follows: Section II is devoted to the noise-free stochastic process, the definition of its joint probability density and expressions for the moments of this density in terms of a Taylor-Itô expansion. Section III provides the properties of the measurement noise under consideration and in section IV expressions for the moments of a noisy process will be derived. After looking at the benefits of equidistantly sampled experimental time series in section V, the previously derived expressions will be used in section VI to extract the parameters of the measurement noise and in section VII to extract polynomial approximations for drift and diffusion functions. Finally in section VIII the results will be applied to some synthetic time series. The used properties of the Gauss function and further computational details are given in appendices A and B.

II. STOCHASTIC PROCESS

Let $\mathbf{X}(t)$ be a stochastic process in N dimensions that can be described by a time-independent Itô -Langevin equation

$$d\mathbf{X}_i(t) = \mathbf{D}^{(1)}(\mathbf{X}) dt + \sqrt{\mathbf{D}^{(2)}(\mathbf{X})} d\mathbf{W}(t), \quad (1)$$

where $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ are the Kramers-Moyal coefficients of the corresponding Fokker-Planck equation and $d\mathbf{W}$ denotes a vector of increments of independent Wiener processes with $\langle dW_i dW_j \rangle = \delta_{ij} dt$. The notation $\sqrt{\mathbf{D}^{(2)}}$ is used to denote a matrix \mathbf{g} with $\mathbf{g} \cdot \mathbf{g}^t = \mathbf{D}^{(2)}$ [31].

Let the one- and two-point probability density functions of

\mathbf{X} be denoted by

$$\rho(\mathbf{x}) := p(\mathbf{x}, t) \quad (2a)$$

$$\rho(\mathbf{x}, \mathbf{x}', \tau) := p(\mathbf{x}, t; \mathbf{x}', t + \tau) \quad (2b)$$

$$= \rho(\mathbf{x}) p(\mathbf{x}', t + \tau | \mathbf{x}, t) \quad (2c)$$

and let the conditioned moments of $\rho(\mathbf{x}, \mathbf{x}', \tau)$ be defined as follows (the notation $d\mathbf{x}$ is used to denote the product $dx_1 \dots dx_N$ whereas $d\mathbf{x}$ denotes a vector of differentials dx_i).

$$m^{(0)}(\mathbf{x}) = \int_{\mathbf{x}'} \rho(\mathbf{x}, \mathbf{x}', \tau) d\mathbf{x}' \quad (3a)$$

$$m_i^{(1)}(\mathbf{x}, \tau) = \int_{\mathbf{x}'} (x'_i - x_i) \rho(\mathbf{x}, \mathbf{x}', \tau) d\mathbf{x}' \quad (3b)$$

$$m_{ij}^{(2)}(\mathbf{x}, \tau) = \int_{\mathbf{x}'} (x'_i - x_i)(x'_j - x_j) \rho(\mathbf{x}, \mathbf{x}', \tau) d\mathbf{x}' \quad (3c)$$

These moments are observable quantities. For a given time series they can be estimated by binning or other density-estimation techniques. Using Eq. (2c) allows to express the moments $\mathbf{m}^{(k)}$ in terms of moments $\mathbf{h}^{(k)}$ of the conditional increments of \mathbf{X}

$$m^{(0)}(\mathbf{x}) = \rho(\mathbf{x}) \cdot 1 \quad (4a)$$

$$m_i^{(1)}(\mathbf{x}, \tau) = \rho(\mathbf{x}) \cdot h_i^{(1)}(\mathbf{x}, \tau) \quad (4b)$$

$$m_{ij}^{(2)}(\mathbf{x}, \tau) = \rho(\mathbf{x}) \cdot h_{ij}^{(2)}(\mathbf{x}, \tau), \quad (4c)$$

with

$$h_i^{(1)}(\mathbf{x}, \tau) := \left. \langle [X_i(t + \tau) - X_i(t)] \right|_{\mathbf{X}(t) = \mathbf{x}} \rangle \quad (5a)$$

$$h_{ij}^{(2)}(\mathbf{x}, \tau) := \left. \langle [X_i(t + \tau) - X_i(t)] \right. \\ \left. \times [X_j(t + \tau) - X_j(t)] \right|_{\mathbf{X}(t) = \mathbf{x}} \rangle. \quad (5b)$$

A Taylor-Itô expansion of Eq. (1) provides expressions for these expectation values. Provided that $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ are smooth functions in \mathbf{x} , it is possible to represent $\mathbf{h}^{(1)}$ and $\mathbf{h}^{(2)}$ as power series in τ . The lowest order terms in these series are linear in τ . The series-coefficients are given by sums of products of the Kramers-Moyal coefficients and their derivatives and are thus generally functions of \mathbf{x} .

$$h_i^{(1)}(\mathbf{x}, \tau) = \sum_{k=1}^{\infty} c_i^{(1,k)}(\mathbf{x}) \tau^k \quad (6a)$$

$$h_{ij}^{(2)}(\mathbf{x}, \tau) = \sum_{k=1}^{\infty} c_{ij}^{(2,k)}(\mathbf{x}) \tau^k \quad (6b)$$

The explicit terms up to second order are given below (using index notation and summation convention). A detailed description of the Taylor-Itô expansion and its moments can be found in [30].

$$h_i^{(1)} = \tau D_i^{(1)} + \frac{\tau^2}{2} \left[D_j^{(1)} \partial_j D_i^{(1)} + \frac{1}{2} D_{jk}^{(2)} \partial_j \partial_k D_i^{(1)} \right] + O(\tau^3) \quad (7a)$$

$$h_{ij}^{(2)} = \tau D_{ij}^{(2)} + \frac{\tau^2}{2} \left[2 D_i^{(1)} D_j^{(1)} + D_{ik}^{(2)} \partial_k D_j^{(1)} + D_{jk}^{(2)} \partial_k D_i^{(1)} + D_k^{(1)} \partial_k D_{ij}^{(2)} + \frac{1}{2} D_{kl}^{(2)} \partial_k \partial_l D_{ij}^{(2)} \right] + O(\tau^3) \quad (7b)$$

Inserting the series representations into Eq. (4) yields a relation between the observable moments $\mathbf{m}^{(k)}$ and the unknown functions $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$. For small values of τ this allows the direct estimation of the Kramers-Moyal coefficients.

$$D_i^{(1)}(\mathbf{x}) = \frac{1}{\tau} \frac{m_i^{(1)}(\mathbf{x}, \tau)}{m^{(0)}(\mathbf{x})} + O(\tau) \quad (8a)$$

$$D_{ij}^{(2)}(\mathbf{x}) = \frac{1}{\tau} \frac{m_{ij}^{(2)}(\mathbf{x}, \tau)}{m^{(0)}(\mathbf{x})} + O(\tau) \quad (8b)$$

III. MEASUREMENT NOISE

The measurement noise under consideration is denoted by $\mathbf{Y}(t)$ and described by an Ornstein-Uhlenbeck process in N dimensions. Such a process is characterized by linear drift- and constant diffusion functions and its statistical properties can be derived analytically (see e.g. [31]). The temporal evolution of \mathbf{Y} is described by Eq. (9). Here the eigenvalues of matrix \mathbf{A} are required to have positive real part and matrix \mathbf{B} is assumed to be symmetric and positive semi-definite. The notation $\sqrt{\mathbf{B}}$ is used to denote a matrix \mathbf{g} with $\mathbf{g} \cdot \mathbf{g}^t = \mathbf{B}$ and the elements of $d\mathbf{W}$ denote the increments of independent Wiener processes with $\langle dW_i dW_j \rangle = \delta_{ij} dt$.

$$d\mathbf{Y}(t) = -\mathbf{A} \cdot \mathbf{Y} dt + \sqrt{\mathbf{B}} d\mathbf{W}(t). \quad (9)$$

While \mathbf{A} and \mathbf{B} are appropriate to describe the temporal evolution of \mathbf{Y} , the 'macroscopic' properties of the noise are more conveniently described in terms of the covariance matrix \mathbf{V} and the matrix of (exponentially decaying) correlation functions $\mathbf{M}(\tau)$. Looking at the auto-covariance of \mathbf{Y} one finds

$$\langle \mathbf{Y}(t + \tau) \mathbf{Y}^t(t) \rangle = \mathbf{M}(\tau) \mathbf{V} \quad (10)$$

with

$$\mathbf{M}(\tau) = e^{-\mathbf{A}\tau} \quad (11)$$

$$\mathbf{V} = \int_0^\infty e^{-\mathbf{A}s} \mathbf{B} e^{-\mathbf{A}^t s} ds. \quad (12)$$

Furthermore \mathbf{Y} is found to be Gaussian distributed. If $G(\mathbf{V}, \mathbf{x})$ is used to denote a normalized Gauss function in \mathbf{x} with covariance \mathbf{V} (see Eq. (A4)), then the one- and two-point probability density functions ρ_Y can be written as

$$\rho_Y(\mathbf{x}) = G(\mathbf{V}, \mathbf{x}) \quad (13a)$$

$$\rho_Y(\mathbf{x}, \mathbf{x}', \tau) = G(\mathbf{V}, \mathbf{x}) G(\mathbf{C}(\tau), \mathbf{x}' - \mathbf{M}(\tau)\mathbf{x}) \quad (13b)$$

with the shortcut

$$\mathbf{C}(\tau) := \mathbf{V} - \mathbf{M}(\tau)\mathbf{V}\mathbf{M}^t(\tau). \quad (14)$$

A note on the eigenvalues of \mathbf{A} and \mathbf{M} : If λ_i denotes the eigenvalues of \mathbf{A} , then the eigenvalues of $\mathbf{M}(\tau)$ are given by $e^{-\lambda_i \tau}$. By introducing the relaxation times (or characteristic time scales) T_i as $T_i := 1/\lambda_i$, the eigenvalues of \mathbf{M} can be written as $e^{-\tau/T_i}$. In the numerical examples given later, the measurement noise will be characterized by such relaxation times T_i instead of by eigenvalues of \mathbf{A} .

IV. NOISY STOCHASTIC PROCESS

Let $\mathbf{X}^*(t) = \mathbf{X}(t) + \mathbf{Y}(t)$ be the sum of a stochastic signal $\mathbf{X}(t)$ and measurement noise $\mathbf{Y}(t)$ as introduced in sections II and III, respectively. Because \mathbf{X} and \mathbf{Y} are independent stochastic variables, the probability density functions of their sum \mathbf{X}^* is given by the convolution of the individual density functions.

$$\begin{aligned} \rho^*(\mathbf{x}, \mathbf{x}', \tau) &= \rho_Y(\mathbf{x}, \mathbf{x}', \tau) * \rho(\mathbf{x}, \mathbf{x}', \tau) \\ &= \int_{\mathbf{z}} \int_{\mathbf{z}'} \rho_Y(\mathbf{x} - \mathbf{z}, \mathbf{x}' - \mathbf{z}', \tau) \\ &\quad \times \rho(\mathbf{z}, \mathbf{z}', \tau) d\mathbf{z} d\mathbf{z}' \end{aligned} \quad (15)$$

Instead of the conditioned moments $\mathbf{m}^{(k)}$ only their noisy counterparts $\mathbf{m}^{*(k)}$ can be determined.

$$m^{*(0)}(\mathbf{x}) = \int_{\mathbf{x}'} \rho^*(\mathbf{x}, \mathbf{x}', \tau) d\mathbf{x}' \quad (16a)$$

$$m_i^{*(1)}(\mathbf{x}, \tau) = \int_{\mathbf{x}'} (x'_i - x_i) \rho^*(\mathbf{x}, \mathbf{x}', \tau) d\mathbf{x}' \quad (16b)$$

$$\begin{aligned} m_{ij}^{*(2)}(\mathbf{x}, \tau) &= \int_{\mathbf{x}'} (x'_i - x_i)(x'_j - x_j) \\ &\quad \times \rho^*(\mathbf{x}, \mathbf{x}', \tau) d\mathbf{x}'. \end{aligned} \quad (16c)$$

Inserting the definitions of ρ^* and ρ_Y (Eqs. (15) and (13b) respectively) and interchanging the order of integration, the

integration with respect to \mathbf{x}' can be performed within the convolution integral. Using the definition of the moments $\mathbf{m}^{(k)}$ and taking advantage of the properties of the Gauss function then finally leads to the following equations (see appendix B). Function arguments are omitted for notational simplicity.

$$m^{*(0)} = \rho_Y * m^{(0)} \quad (17a)$$

$$m_i^{*(1)} = \rho_Y * (h_i^{(1)} m^{(0)}) + Q_{ii'} \partial_{i'} m^{*(0)} \quad (17b)$$

$$\begin{aligned} m_{ij}^{*(2)} &= \rho_Y * (h_{ij}^{(2)} m^{(0)}) \\ &\quad + (Q_{ij} + Q_{ji} - Q_{ii'} Q_{jj'} \partial_{i'} \partial_{j'}) m^{*(0)} \\ &\quad + Q_{ii'} \partial_{i'} m_j^{*(1)} + Q_{jj'} \partial_{j'} m_i^{*(1)} \end{aligned} \quad (17c)$$

Here $\rho_Y(\mathbf{x}) = G(\mathbf{V}, \mathbf{x})$ is the density function of the measurement noise \mathbf{Y} . The terms $\mathbf{h}^{(k)}$, as introduced in section II, denote the moments of the conditional increments of \mathbf{X} . The quantity \mathbf{Q} , finally, has been introduced as an abbreviation and is defined as

$$\mathbf{Q}(\tau) := (\mathbf{Id} - \mathbf{M}(\tau))\mathbf{V}. \quad (18)$$

Equation (17) allows to express the observable moments $\mathbf{m}^{*(k)}$ in terms of the unknowns $m^{(0)}$, $\mathbf{h}^{(k)}$, \mathbf{M} and \mathbf{V} . However it is possible to use Eq. (17b) to extract the parameters of the measurement noise without the need for a simultaneous determination of $\mathbf{h}^{(k)}$ and $m^{(0)}$. This will be done in section VI. Next, however, an assumption on the given time series will be made.

V. EXPERIMENTAL TIME SERIES

It will be assumed, that the values of a given time series are taken at equidistant points in time with a basic time increment of Δt . This is often assumed tacitly but shall be stated here explicitly because it will be used in the following.

$$\mathbf{X}_i^* := \mathbf{X}^*(i\Delta t), \quad i = 1, \dots, i_{\max} \quad (19)$$

Increments of \mathbf{X}^* can thus be calculated for all time increments τ which are integral multiples of Δt . The experimental two-point probability density $\tilde{\rho}^*(\mathbf{x}, \mathbf{x}', \tau)$ for those values of τ can then be written as a sum of Dirac-distributions.

$$\begin{aligned} \tilde{\rho}^*(\mathbf{x}, \mathbf{x}', k\Delta t) &= \frac{1}{i_{\max} - k} \sum_{i=1}^{i_{\max}-k} \delta(\mathbf{x} - \mathbf{X}_i^*) \\ &\quad \times \delta(\mathbf{x}' - \mathbf{X}_{i+k}^*) \end{aligned} \quad (20)$$

Weighted integrals of the 'true' density ρ^* can easily be estimated by weighted integrals of $\tilde{\rho}^*$ now. Given a weight function $f(\mathbf{x}, \mathbf{x}')$ and denoting the estimate by \tilde{I} one finds

$$\tilde{I} = \int_{\mathbf{x}} \int_{\mathbf{x}'} f(\mathbf{x}, \mathbf{x}') \tilde{\rho}^*(\mathbf{x}, \mathbf{x}', k\Delta t) d\mathbf{x} d\mathbf{x}'$$

$$= \frac{1}{i_{\max} - k} \sum_{i=1}^{i_{\max}-k} f(\mathbf{X}_i^*, \mathbf{X}_{i+k}^*). \quad (21)$$

Weighted integrals of ρ^* can therefore directly be estimated from the given time series. There is no need to use binning to estimate the density ρ^* first [29]. Weighted integrals of the moments $\mathbf{m}^{*(k)}$ can be treated the same way by expressing them as weighted integrals of ρ^* using Eq. (16).

VI. EXTRACTING MEASUREMENT NOISE PARAMETERS

Multiplying Eq. (17b) by x_j and subsequently applying an integration with respect to \mathbf{x} leads to

$$\int_{\mathbf{x}} m_i^{*(1)} x_j d\mathbf{x} = \int_{\mathbf{x}} [\rho_Y * (h_i^{(1)} m^{(0)})] x_j d\mathbf{x} + Q_{ii'} \int_{\mathbf{x}} (\partial_{i'} m^{*(0)}) x_j d\mathbf{x}. \quad (22)$$

The left hand side of this equation can directly be estimated from a given time series and will be denoted by \mathbf{Z} .

$$Z_{ij}(\tau) := \int_{\mathbf{x}} m_i^{*(1)}(\mathbf{x}, \tau) x_j d\mathbf{x} \quad (23)$$

Applying integration by parts allows the evaluation of the second integral on the right hand side

$$Q_{ii'} \int_{\mathbf{x}} (\partial_{i'} m^{*(0)}) x_j d\mathbf{x} = -Q_{ij}. \quad (24)$$

The remaining integral in Eq. (22) only depends on τ because of the function $\mathbf{h}^{(1)}(\mathbf{x}, \tau)$. Using Eq. (6a) therefore allows to express the integral as a power series in τ with unknown coefficients $P_{ij}^{(\nu)}$. Truncating this series to some order ν_{\max} yields an approximation of the integral by a polynomial in τ .

$$\int_{\mathbf{x}} [\rho_Y * (h_i^{(1)} m^{(0)})] x_j d\mathbf{x} = \sum_{\nu=1}^{\nu_{\max}} P_{ij}^{(\nu)} \tau^{\nu} \quad (25)$$

Putting this all together (and additionally replacing the abbreviation \mathbf{Q} by its definition) so far yields

$$\mathbf{Z}(\tau) = \sum_{\nu=1}^{\nu_{\max}} \mathbf{P}^{(\nu)} \tau^{\nu} - (\mathbf{Id} - \mathbf{M}(\tau)) \mathbf{V}. \quad (26)$$

Assuming that the time series is sampled with a basic time increment Δt (as stated in section V), the value of $\mathbf{Z}(\tau)$ can directly be estimated for all increments τ being integral multiples of Δt . The corresponding value of \mathbf{M} is given by an

integral power of $\mathbf{M}(\Delta t)$ then. This is due to the fact that $\mathbf{M}(\tau)$ (according to section III) is a matrix exponential.

$$\mathbf{M}_0 := \mathbf{M}(\Delta t) = e^{-\mathbf{A}\Delta t} \quad (27a)$$

$$\Rightarrow \mathbf{M}(k\Delta t) = e^{-\mathbf{A}k\Delta t} = \mathbf{M}_0^k \quad (27b)$$

So finally one gets

$$\mathbf{Z}(k\Delta t) = \sum_{\nu=1}^{\nu_{\max}} \mathbf{P}^{(\nu)} (k\Delta t)^{\nu} - (\mathbf{Id} - \mathbf{M}_0^k) \mathbf{V}. \quad (28)$$

Evaluating \mathbf{Z} for a sufficient number of increments, $k\Delta t$, yields a system of equations that can (iteratively) be solved for the unknowns $\mathbf{P}^{(\nu)}$, \mathbf{V} and \mathbf{M}_0 in a least square sense. Subsequently the relaxation times of the measurement noise, T_i , can be calculated from the eigenvalues of \mathbf{M}_0 .

For such a fit to succeed, two conditions must be met.

- Firstly, the largest increment $k_{\max}\Delta t$ should be small compared to the characteristic time scale of the underlying stochastic process. This will allow, to chose a low polynomial order ν_{\max} (the smaller τ the better $\mathbf{h}^{(1)}$ can be approximated by low order polynomials).
- Secondly, the relaxation times T_i should be small compared to $k_{\max}\Delta t$. This will allow, to distinguish the exponential functions in $\mathbf{M}(\tau)$ from a low order polynomial.

The proposed method is therefore limited to measurement noise with relaxation times T_i considerably smaller than the time scale of the underlying stochastic process.

VII. EXTRACTING DRIFT- AND DIFFUSION FUNCTIONS

In the following it will be assumed, that the noise parameters have already been estimated according to section VI. The parameters and derived quantities like $\mathbf{Q}(\tau)$ will therefore be treated as known quantities.

Multiplying Eqs. (17b) and (17c) by some weight function $\Psi(\mathbf{x})$ and subsequently applying an integration with respect to \mathbf{x} yields

$$\text{lhs}_i = \int_{\mathbf{x}} \Psi \left[\rho_Y * (h_i^{(1)} m^{(0)}) \right] d\mathbf{x} \quad (29a)$$

$$\text{lhs}_{ij} = \int_{\mathbf{x}} \Psi \left[\rho_Y * (h_{ij}^{(2)} m^{(0)}) \right] d\mathbf{x} \quad (29b)$$

where lhs_i and lhs_{ij} are abbreviations for the left hand sides

$$\text{lhs}_i := \int_{\mathbf{x}} \Psi \left[m_i^{*(1)} - Q_{ii'} \partial_{i'} m^{*(0)} \right] d\mathbf{x} \quad (30a)$$

$$\text{lhs}_{ij} := \int_{\mathbf{x}} \Psi \left[m_{ij}^{*(2)} - (Q_{ij} + Q_{ji}) \right] d\mathbf{x}$$

$$\begin{aligned} & -Q_{ii'}Q_{jj'}\partial_{i'}\partial_{j'}m^{*(0)} \\ & -Q_{ii'}\partial_{i'}m_j^{*(1)} - Q_{jj'}\partial_{j'}m_i^{*(1)} \Big] dx. \end{aligned} \quad (30b)$$

Applying integration by parts allows to express the integrals in Eq. (30) as sums of weighted integrals of $m^{*(k)}$. For example one finds $\int \Psi m_i^{*(1)} + Q_{ii'} \int (\partial_{i'} \Psi) m^{*(0)}$ for the left hand side of Eq. (29a). This expression can directly be estimated from the given time series because \mathbf{Q} and Ψ (and thus also the derivatives of Ψ) are known. The same holds for the left hand side of Eq. (29b). Both left hand sides can therefore directly be estimated for a given choice of τ and Ψ .

The corresponding right hand sides, however, refer to the unknown function $m^{(0)}$. It is possible to overcome this problem if the drift- and diffusion functions are approximated by polynomials in \mathbf{x} .

$$D_i^{(1)} = a_i^{(1)} + a_{i\alpha}^{(1)}x_\alpha + a_{i\alpha\beta}^{(1)}x_\alpha x_\beta + \dots \quad (31a)$$

$$D_{ij}^{(2)} = a_{ij}^{(2)} + a_{ij\alpha}^{(2)}x_\alpha + a_{ij\alpha\beta}^{(2)}x_\alpha x_\beta + \dots \quad (31b)$$

The coefficients in the power series representation of the conditional moments $\mathbf{h}^{(k)}$ then also become polynomials in \mathbf{x} .

$$\begin{aligned} h_i^{(1)} = & \tau \left[a_i^{(1)} + a_{i\alpha}^{(1)}x_\alpha + a_{i\alpha\beta}^{(1)}x_\alpha x_\beta + \dots \right] \\ & + \tau^2 \left[b_i^{(1)} + b_{i\alpha}^{(1)}x_\alpha + b_{i\alpha\beta}^{(1)}x_\alpha x_\beta + \dots \right] \\ & + \dots \end{aligned} \quad (32a)$$

$$\begin{aligned} h_{ij}^{(2)} = & \tau \left[a_{ij}^{(2)} + a_{ij\alpha}^{(2)}x_\alpha + a_{ij\alpha\beta}^{(2)}x_\alpha x_\beta + \dots \right] \\ & + \tau^2 \left[b_{ij}^{(2)} + b_{ij\alpha}^{(2)}x_\alpha + b_{ij\alpha\beta}^{(2)}x_\alpha x_\beta + \dots \right] \\ & + \dots \end{aligned} \quad (32b)$$

For the sake of simplicity the abbreviations $\mathbf{b}^{(k)}$ have been introduced here. However all the coefficients in Eq. (32) can of course be expressed in terms of the coefficients $\mathbf{a}^{(k)}$. Using Eq. (32) the problem of expressing the right hand sides of Eq. (29) reduces to the problem of expressing terms of the form

$$F_{\alpha_1 \dots \alpha_k} := \int_{\mathbf{x}} \Psi \left[\rho_Y * (x_{\alpha_1} \dots x_{\alpha_k} m^{(0)}) \right] dx. \quad (33)$$

Because $\rho_Y = G(\mathbf{V}, \mathbf{x})$ is a Gauss function, the convolution within the square brackets can be expressed in terms of derivatives of $m^{*(0)}$, $x_\alpha m^{*(0)}$, $x_\alpha x_\beta m^{*(0)}$, ... (see appendix A 5). One finds

$$\begin{aligned} \rho_Y * [m^{(0)}] &= m^{*(0)} \\ \rho_Y * [x_\alpha m^{(0)}] &= x_\alpha m^{*(0)} + L_\alpha m^{*(0)} \\ \rho_Y * [x_\alpha x_\beta m^{(0)}] &= x_\alpha x_\beta m^{*(0)} + L_\alpha [x_\beta m^{*(0)}] \\ &\quad + L_\beta [x_\alpha m^{*(0)}] + L_{\alpha\beta} m^{*(0)} \\ &\vdots \end{aligned} \quad (34)$$

with the linear differential operators

$$\begin{aligned} L_\alpha &= V_{\alpha\alpha'} \partial_{\alpha'} \\ L_{\alpha\beta} &= V_{\alpha\alpha'} V_{\beta\beta'} \partial_{\alpha'} \partial_{\beta'} - V_{\alpha\beta} \\ &\vdots \end{aligned} \quad (35)$$

Applying integration by parts then allows to express Eq. (33) in terms of weighted integrals of $m^{*(0)}$, which can directly be estimated from the given time series. One finds

$$\begin{aligned} F &= \int_{\mathbf{x}} \Psi m^{*(0)} dx \\ F_\alpha &= \int_{\mathbf{x}} \left\{ \Psi x_\alpha m^{*(0)} - [L_\alpha \Psi] m^{*(0)} \right\} dx \\ F_{\alpha\beta} &= \int_{\mathbf{x}} \left\{ \Psi x_\alpha x_\beta m^{*(0)} - [L_\alpha \Psi] x_\beta m^{*(0)} \right. \\ &\quad \left. - [L_\beta \Psi] x_\alpha m^{*(0)} + [L_{\alpha\beta} \Psi] m^{*(0)} \right\} dx \\ &\vdots \end{aligned} \quad (36)$$

Expressing the right hand sides of Eq. (29) in terms of F, F_α, \dots one finally obtains the following equations.

$$\begin{aligned} \text{lhs}_i = & \tau \left[a_i^{(1)} F + a_{i\alpha}^{(1)} F_\alpha + a_{i\alpha\beta}^{(1)} F_{\alpha\beta} + \dots \right] \\ & + \tau^2 \left[b_i^{(1)} F + b_{i\alpha}^{(1)} F_\alpha + b_{i\alpha\beta}^{(1)} F_{\alpha\beta} + \dots \right] \\ & + \dots \end{aligned} \quad (37a)$$

$$\begin{aligned} \text{lhs}_{ij} = & \tau \left[a_{ij}^{(2)} F + a_{ij\alpha}^{(2)} F_\alpha + a_{ij\alpha\beta}^{(2)} F_{\alpha\beta} + \dots \right] \\ & + \tau^2 \left[b_{ij}^{(2)} F + b_{ij\alpha}^{(2)} F_\alpha + b_{ij\alpha\beta}^{(2)} F_{\alpha\beta} + \dots \right] \\ & + \dots \end{aligned} \quad (37b)$$

Evaluating the left hand sides and the quantities F, F_α, \dots for a sufficient number of increments τ and weight functions Ψ yields a system of equations that can be solved for the unknown polynomial coefficients in a least square sense. There are different approaches to deal with the higher order terms in τ now.

- The most simple approach is, to completely ignore the higher order terms. This will lead to a linear fit in τ . Furthermore the resulting set of equations will be linear in the unknown coefficients $\mathbf{a}^{(k)}$.
- A more elaborate approach is, to perform a polynomial fit in τ . Coefficients beyond some order will be ignored. If the remaining coefficients are treated as additional unknowns, then the resulting set of equations will stay linear. However this way some available information is ignored, because $\mathbf{b}^{(k)}$ and higher order coefficients can in fact be expressed in terms of the coefficients $\mathbf{a}^{(k)}$.
- Finally, a polynomial fit in τ can be performed, where the higher order coefficients are expressed in terms of the coefficients $\mathbf{a}^{(k)}$. This will improve the accuracy

of the estimate, because of the smaller number of unknowns. The resulting set of equations, however, will now be nonlinear and needs to be solved iteratively.

The choice of the weight functions Ψ has been left open up to now. Obviously Ψ needs to admit the various integrations by parts that have been applied. For these integrations it also has been tacitly assumed that the involved boundary values at $|\mathbf{x}| \rightarrow \infty$ are vanishing. This imposes additional restrictions on Ψ .

The set of weight functions used in the numerical examples, given below, consisted of a number of Gauss functions centered at different points in space. There may be better choices, but the problem of finding the 'best' set of functions will not be addressed here. Gauss functions are smooth and real valued and have a local support. But maybe it would be better to choose, for example, some complex valued functions like $\exp(i\omega^t \mathbf{x})$ which have a local support in Fourier space only. Also piecewise polynomial functions like the B-spline base functions may be an alternative.

VIII. APPLICATION TO NUMERICAL DATA

In order to check the accuracy of the proposed method, a test case in two dimensions has been investigated. A stochastic process, $\mathbf{X}(t)$, as introduced in Sec. II, has been specified by the following choice for the drift- and diffusion functions (x and y denote the components of the vector \mathbf{x}).

$$\mathbf{D}^{(1)}(\mathbf{x}) = \begin{pmatrix} x - xy \\ x^2 - y \end{pmatrix} \quad (38a)$$

$$\mathbf{D}^{(2)}(\mathbf{x}) = \begin{pmatrix} 0.5 & 0 \\ 0 & 0.5(1 + x^2) \end{pmatrix} \quad (38b)$$

By numerical integration synthetic time series of the process can be generated. All series used in the following will consist of 10^7 points, sampled at time increments $\Delta t = 0.005$. The deterministic part of the process dynamic and the experimental density distribution of \mathbf{X} is visualized in Fig. 1.

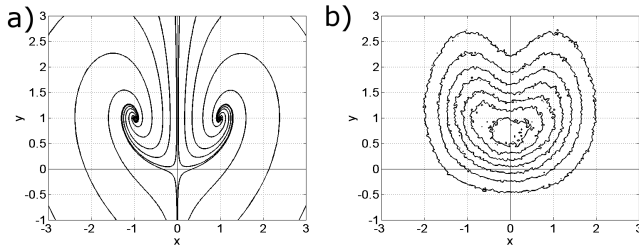


FIG. 1: Deterministic dynamic and density distribution of the 2D process $\mathbf{X}(t)$. The trajectories in phase space (a) are generated by the deterministic part of the process dynamic ($\dot{x} = x - xy$, $\dot{y} = x^2 - y$). There exist three fixed points: a saddle at the origin and two stable foci at $(x = \pm 1, y = 1)$. The contour lines (b) of the probability density function have been computed from a time series of \mathbf{X} .

The measurement noise, $\mathbf{Y}(t)$, as introduced in Sec. III, is described by an Ornstein-Uhlenbeck process in two dimensions. The noise is characterized by eigen-directions, $\mathbf{e}_{i\mathbf{M}}$, and corresponding relaxation times, T_i , of its matrix \mathbf{M} and by the principal directions, $\mathbf{e}_{i\mathbf{V}}$, and the corresponding standard deviations, σ_i , of its covariance matrix \mathbf{V} . The following values have been chosen (relaxation times are given in units of Δt).

$$(\mathbf{e}_1, \mathbf{e}_2)_{\mathbf{M}} = \begin{pmatrix} 1 & 1 \\ 0 & 2 \end{pmatrix}, \quad \mathbf{T} = \begin{pmatrix} 1 \\ 3 \end{pmatrix} \quad (39a)$$

$$(\mathbf{e}_1, \mathbf{e}_2)_{\mathbf{V}} = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad \boldsymbol{\sigma} = \begin{pmatrix} 0.25 \\ 0.5 \end{pmatrix} \quad (39b)$$

The deterministic part of the dynamic of the measurement noise and the experimental density distribution of \mathbf{Y} is visualized in Fig. 2.

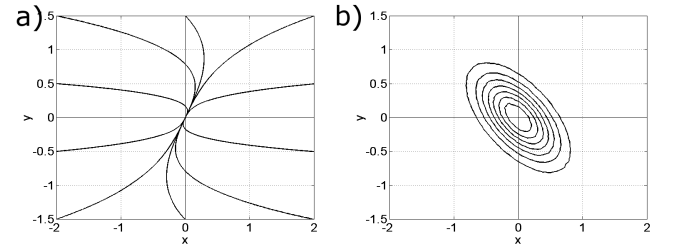


FIG. 2: Deterministic dynamic and density distribution of the 2D measurement noise $\mathbf{Y}(t)$. The trajectories in phase space (a) are generated by the deterministic part of the process dynamic ($\dot{x} = -x + y/3$, $\dot{y} = -y/3$). There exists a single, attractive, fixed point at the origin. The contour lines (b) of the probability density function have been computed from a time series of \mathbf{Y} .

Adding the time series of \mathbf{X} and \mathbf{Y} yields a series of 'noisy' values $\mathbf{X}^*(t) = \mathbf{X}(t) + \mathbf{Y}(t)$. This will be called a noisy time series in the following. Excerpts of $\mathbf{X}(t)$ and $\mathbf{X}^*(t)$ as well as the experimental density distribution of \mathbf{X}^* are shown in Fig. 3.

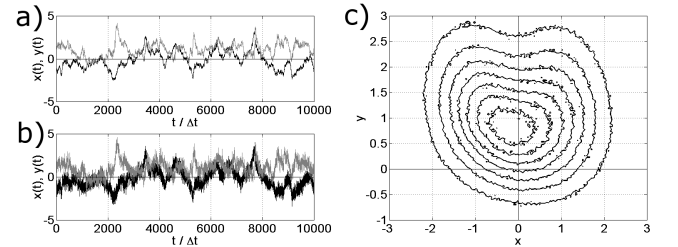


FIG. 3: Excerpt of a time series of $\mathbf{X}(t)$ (a) and of a corresponding noisy time series of $\mathbf{X}^*(t)$ (b). The contour lines (c) of the probability density function have been computed from a noisy time series.

Now the extraction of the measurement noise parameters, as described in Sec. VI, has been tested. For a sample of

1000 independent realizations of noisy time series the matrices $\mathbf{M}(\Delta t)$ and \mathbf{V} have been estimated. For each estimate a number of scalar quantities has been calculated. For a characterization of the deterministic part of the noise-dynamic the angles, α_i , spanned by the eigendirections of \mathbf{M} and the x -axis, and the relaxation times, T_i , determined by the eigenvalues of $\mathbf{M}(\Delta t)$, have been used. Their true values are given by

$$\alpha_1 = 0^\circ, \quad \alpha_2 \approx 63.43^\circ \quad (40a)$$

$$T_1/\Delta t = 1, \quad T_2/\Delta t = 3 \quad (40b)$$

The covariance matrix \mathbf{V} is symmetric and can thus be characterized by three scalars: the angle β , spanned by the first principal direction of \mathbf{V} and the x -axis, and the standard deviations σ_i in direction of the principal axes. The true values are given by

$$\beta = 45^\circ \quad (41a)$$

$$\sigma_1 = 0.25, \quad \sigma_2 = 0.5 \quad (41b)$$

Parameter fitting has been performed with a maximum increment $\tau_{\max} = 50\Delta t$ and a maximum polynomial order of $\nu_{\max} = 3$. The resulting distributions of the estimates are shown in Figs. 4 and 5. It turns out, that the sample standard deviations of the angular quantities are given by some tenth of a degree. Relaxation times and noise strengthes are estimated with relative errors well below one percent.

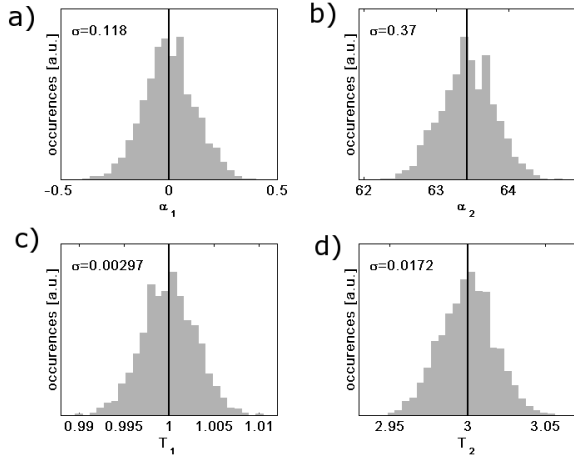


FIG. 4: Histograms of the observed distributions of the estimated parameters characterizing matrix \mathbf{M} of the 2D measurement noise. Angles α_i of the eigen-directions (a,b) and corresponding relaxation times T_i in units of Δt (c,d). The standard deviation of the respective distribution is given by an annotation. The true parameter values are indicated by solid vertical lines.

For the estimation of the drift- and diffusion functions a complete quadratic ansatz has been made for each component of $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$. Because $\mathbf{D}^{(2)}$ is symmetric, this leads to a

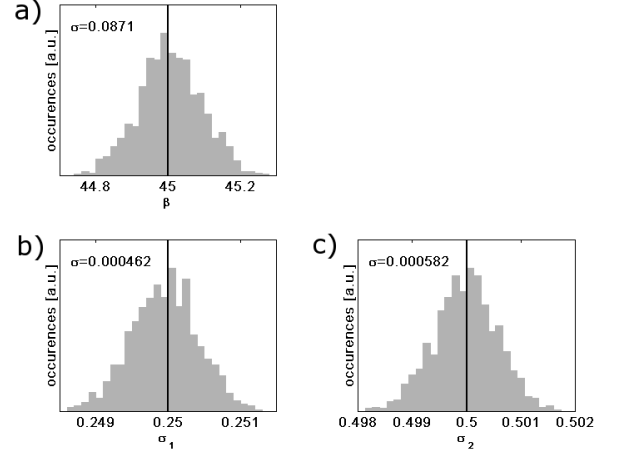


FIG. 5: Histograms of the observed distributions of the estimated parameters characterizing the covariance matrix \mathbf{V} of the 2D measurement noise. Angle β of the first principal direction (a) and the principal standard deviations σ_i (b,c). The standard deviation of the respective distribution is given by an annotation. The true parameter values are indicated by solid vertical lines.

total of 30 coefficients. As maximum time increment for the fitting procedure a value of $\tau_{\max} = 15\Delta t$ has been chosen. The set of weight functions Ψ consisted of 16 Gaussian functions centered at the nodes of a rectangular 4×4 grid covering the $\pm 2\sigma$ range of the experimental density distribution of \mathbf{X}^* . The standard deviations of the weight functions itself was chosen as twice the distance between neighbouring nodes.

For this setup the coefficients have been estimated now for a sample of ten independent realizations of the noisy time series. Using a linear fit in τ leads to the results shown in Figs. 6 and 7.

It can be seen that some of the estimates, especially for the coefficients of the diffusion functions, are significantly biased. Looking, for example, at coefficient a_2 of diffusion function $D_{11}^{(2)}$ one finds a value of -0.1663 ± 0.0097 which significantly differs from the true value of zero. Much better results are obtained by performing a quadratic fit in τ . To do so, the most simple approach has been chosen: For each parameter a_α an additional parameter b_α (see Eq. (37)) is introduced. The only purpose of this parameters is, to absorb some of the quadratic terms in τ . Because the number of unknowns is doubled this way, this will also lead to higher fluctuations of the estimates. However, performing such a quadratic fit also greatly reduces their biasing, as can be seen in Figs. 8 and 9. For the above mentioned coefficient a_2 of $D_{11}^{(2)}$, e.g., one now obtains a value of 0.0025 ± 0.0352 .

The extraction of noise and process parameters from a noisy time series seems to work for the given 2D test case. To check if this also holds for higher dimensions, the test case has been extended to four dimensions. Process and measurement noise

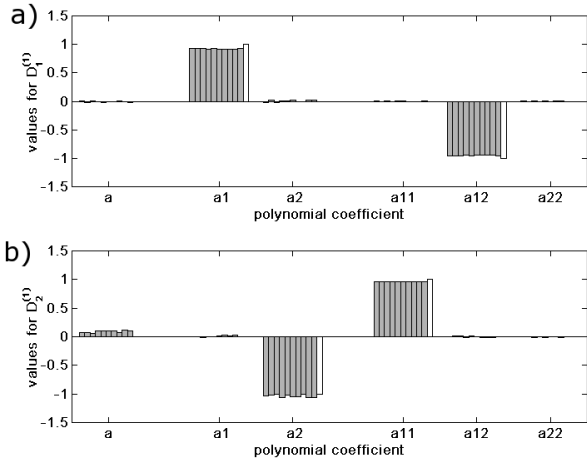


FIG. 6: Parameter estimates for the drift functions $D_1^{(1)}$ (a) and $D_2^{(1)}$ (b) of the 2D process, obtained by a linear fit in τ . For each polynomial coefficient the calculated estimates are given by grey bars with an additional white bar to the right, which shows the true value.

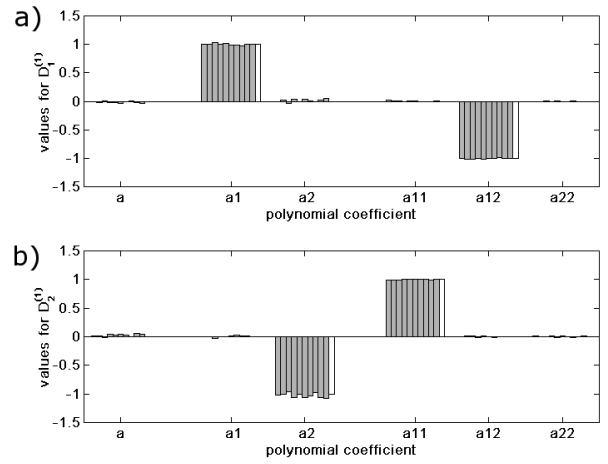


FIG. 8: Parameter estimates for the drift functions $D_1^{(1)}$ (a) and $D_2^{(1)}$ (b) of the 2D process, obtained by a quadratic fit in τ . For each polynomial coefficient the calculated estimates are given by grey bars with an additional white bar to the right, which shows the true value.

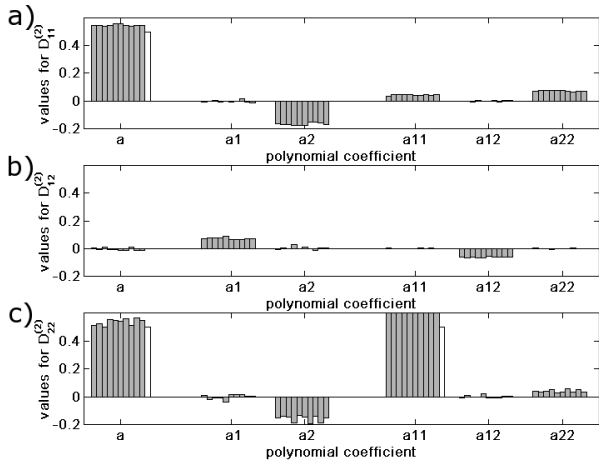


FIG. 7: Parameter estimates for the diffusion functions $D_{11}^{(2)}$ (a), $D_{12}^{(2)}$ (b) and $D_{22}^{(2)}$ (c) of the 2D process, obtained by a linear fit in τ . For each polynomial coefficient the calculated estimates are given by grey bars with an additional white bar to the right, which shows the true value.

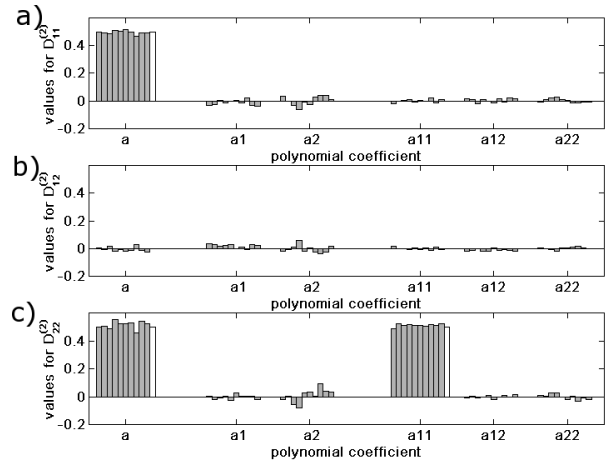


FIG. 9: Parameter estimates for the diffusion functions $D_{11}^{(2)}$ (a), $D_{12}^{(2)}$ (b) and $D_{22}^{(2)}$ (c) of the 2D process, obtained by a quadratic fit in τ . For each polynomial coefficient the calculated estimates are given by grey bars with an additional white bar to the right, which shows the true value.

now are defined in x, y, z, w space. The process is defined by

$$\mathbf{D}^{(1)}(\mathbf{x}) = \begin{pmatrix} x - xy \\ x^2 - y \\ -z \\ -w \end{pmatrix} \quad (42a)$$

$$\mathbf{D}^{(2)}(\mathbf{x}) = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1+x^2}{2} & 0 & 0 \\ 0 & 0 & \frac{1+x^2}{2} & 0 \\ 0 & 0 & 0 & \frac{1+x^2}{2} \end{pmatrix} \quad (42b)$$

and the measurement noise by

$$(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4)_{\mathbf{M}} = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (43a)$$

$$(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4)_{\mathbf{V}} = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (43b)$$

$$\mathbf{T} = \begin{pmatrix} 1 \\ 3 \\ 2 \\ 2 \end{pmatrix}, \quad \boldsymbol{\sigma} = \begin{pmatrix} 0.25 \\ 0.5 \\ 0.25 \\ 0.25 \end{pmatrix}. \quad (44)$$

Estimating the relaxation times and the noise strengthes for a noisy time series (10^7 points, $\Delta t = 0.005$, $\tau_{\max} = 50$, $\nu_{\max} = 3$) yields the following results.

$$\tilde{\mathbf{T}} = \begin{pmatrix} 1.000 \\ 3.009 \\ 1.997 \\ 1.986 \end{pmatrix}, \quad \tilde{\boldsymbol{\sigma}} = \begin{pmatrix} 0.2503 \\ 0.5008 \\ 0.2498 \\ 0.2491 \end{pmatrix} \quad (45)$$

The accuracy of the estimated matrices, $\tilde{\mathbf{M}}$ and $\tilde{\mathbf{V}}$, can be expressed in terms of the relative errors $\epsilon_{\mathbf{M}}$ and $\epsilon_{\mathbf{V}}$, defined as $\mathbf{M}^{-1}\tilde{\mathbf{M}} - \mathbf{Id}$ and $\mathbf{V}^{-1}\tilde{\mathbf{V}} - \mathbf{Id}$ respectively. One finds

$$\epsilon_{\mathbf{M}} = \begin{pmatrix} +0.6 & -5.2 & -5.2 & +2.4 \\ +0.2 & +0.8 & +2.2 & -1.4 \\ +0.5 & +0.8 & -3.0 & +0.8 \\ -1.0 & -1.5 & +2.0 & -1.5 \end{pmatrix} \times 10^{-3} \quad (46a)$$

$$\epsilon_{\mathbf{V}} = \begin{pmatrix} +0.7 & -0.6 & +0.7 & -1.7 \\ -2.1 & +3.1 & +1.8 & -2.5 \\ -0.8 & +3.3 & -5.0 & +1.9 \\ -0.5 & -3.8 & +1.9 & -1.4 \end{pmatrix} \times 10^{-3}. \quad (46b)$$

For the estimation of the drift- and diffusion functions a complete quadratic ansatz has been made for each component of $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$. In four dimensions this leads to a total of 210 coefficients. As maximum time increment for the fitting procedure a value of $\tau_{\max} = 15\Delta t$ has been chosen. The set of

weight functions Ψ consisted of 81 Gaussian functions centered at the nodes of a rectangular $3 \times 3 \times 3 \times 3$ grid covering the $\pm 2\sigma$ range of the experimental density distribution of \mathbf{X}^* . The standard deviations of the weight functions itself was chosen as twice the distance between neighbouring nodes. Using the same type of quadratic fit in τ as in the 2D case yields the coefficient estimates shown in Fig. 10.

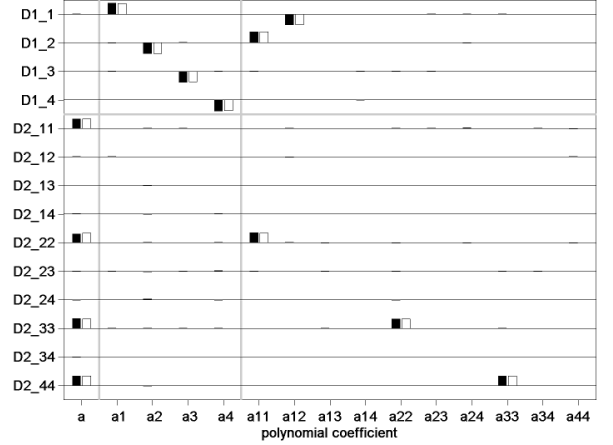


FIG. 10: Parameter estimates for the polynomial coefficients of the drift- and diffusion functions of the 4D process, obtained by a quadratic fit in τ . For each coefficient the calculated estimate is given by a black bar. White bars show the respective true values. Black horizontal lines show the abscissa of the coordinate systems of the respective Drift- and Diffusion functions denoted to the left. The results for constant-, linear- and quadratic coefficients as well as the results for drift- and diffusion functions are separated by grey lines.

IX. CONCLUSIONS

A procedure has been described for the analysis of stochastic time series in N dimensions in the presence of strong measurement noise. The algorithm is able to cope with exponentially correlated noise and accurately extracts strength and correlation time of the measurement noise as well as the parameters defining the drift- and diffusion functions of the underlying stochastic process. This has been shown by the analysis of synthetically generated time series in two and in four dimensions.

The ability to deal with exponentially correlated measurement noise in more than one dimension has not been given by the approaches available up to now.

Because of the use of weight functions there is no need to perform any density binning. All required quantities can be obtained from weighted sums of the values of the time series. This avoids the aliasing errors caused by finite bin sizes.

All calculation have been performed on a standard desktop PC. The analysis of a signal took about five minutes (2D case) respectively fifty minutes (4D case).

In the current implementation only a simplified quadratic fit in the increments τ can be performed. Implementing a full polynomial fit, as mentioned in Sec. VII, should allow to extend the range of time increments that can be used for the analysis and thus should increase the accuracy of the results. This has to be done in the future.

Another point to be improved is the restriction on polynomial approximations of the drift- and diffusion functions. An approximation by spline-based functions would be much more flexible. When using such a parametrization, however, it will no longer be possible to accurately express the convolutions in Eq. (29) in terms of observable quantities. It will become necessary to also introduce a parametrization for the density $m^{(0)}$ which significantly complicates the calculations and also introduces additional parameters to be estimated.

Also a future task is the application to some real world data.

X. ACKNOWLEDGEMENTS

The author especially wants to thank Joachim Peinke, Rudolf Friedrich, Maria Haase, David Kleinhans and Pedro G. Lind for useful discussions.

Appendix A: Gauss functions

1. Index-vectors and monomials

For the sake of a compact syntax, multiple indices will frequently be combined into an index-vector. For example $A_{j_1 \dots j_n}$ will be written as $A_{\mathbf{j}}$. To denote the length of such a vector \mathbf{j} , the function $\ell(\mathbf{j})$ will be used.

As a further abbreviation the symbol \mathcal{M} is introduced for monomials of the components of a vector. A monomial $x_{j_1} \dots x_{j_n}$ will be written as $\mathcal{M}_{j_1 \dots j_n}(\mathbf{x})$ or simply as $\mathcal{M}_{\mathbf{j}}(\mathbf{x})$. Monomials of the nabla vector will be used, to denote multiple partial differentiation more compactly by $\mathcal{M}_{\mathbf{j}}(\nabla)$.

2. Fourier transform and convolution

Let Fourier transform and convolution of functions $\mathbb{R}^N \rightarrow \mathbb{C}$ be defined as below. For notational simplicity the ‘hat’ syntax will be used to denote the Fourier transform of single functions. For more complex expressions the functional form $\mathcal{F}(\dots)$ will usually be the better choice.

$$\mathcal{F}[f(\mathbf{x})](\omega) = \hat{f}(\omega) := \int_{\mathbf{x}} e^{-i\omega^t \mathbf{x}} f(\mathbf{x}) d\mathbf{x} \quad (\text{A1})$$

$$\begin{aligned} f(\mathbf{x}) * g(\mathbf{x}) &:= \int_{\mathbf{x}'} f(\mathbf{x}') g(\mathbf{x} - \mathbf{x}') d\mathbf{x}' \\ &= \int_{\mathbf{x}'} f(\mathbf{x} - \mathbf{x}') g(\mathbf{x}') d\mathbf{x}' \end{aligned} \quad (\text{A2})$$

Above definitions imply the following properties.

$$\mathcal{F}\left[\frac{\partial}{\partial x_j} f(\mathbf{x})\right] = i\omega_j \hat{f}(\omega) \quad (\text{A3a})$$

$$\mathcal{F}[x_j f(\mathbf{x})] = i \frac{\partial}{\partial \omega_j} \hat{f}(\omega) \quad (\text{A3b})$$

$$\mathcal{F}[f(\mathbf{x}) * g(\mathbf{x})] = \hat{f}(\omega) \hat{g}(\omega) \quad (\text{A3c})$$

$$\begin{aligned} \frac{\partial}{\partial x_j} [f(\mathbf{x}) * g(\mathbf{x})] &= \left[\frac{\partial}{\partial x_j} f(\mathbf{x}) \right] * g(\mathbf{x}) \\ &= f(\mathbf{x}) * \left[\frac{\partial}{\partial x_j} g(\mathbf{x}) \right] \end{aligned} \quad (\text{A3d})$$

3. Derivatives and monomial products of Gauss functions

Let $G(\mathbf{C}, \mathbf{x})$ denote a normalized Gauss function with covariance matrix \mathbf{C} and function argument $\mathbf{x} \in \mathbb{R}^N$.

$$G(\mathbf{C}, \mathbf{x}) := \frac{1}{\sqrt{(2\pi)^N |\det(\mathbf{C})|}} e^{-\frac{1}{2} \mathbf{x}^t \mathbf{C}^{-1} \mathbf{x}} \quad (\text{A4})$$

This function is a eigenfunction of the Fourier transform.

$$\begin{aligned} \hat{G}(\mathbf{C}, \omega) &= e^{-\frac{1}{2} \omega^t \mathbf{C} \omega} \\ &= \sqrt{(2\pi)^N |\det(\mathbf{C}^{-1})|} G(\mathbf{C}^{-1}, \omega) \end{aligned} \quad (\text{A5})$$

It can be shown by mathematical induction, that the derivatives of G all have the form

$$\mathcal{M}_{\mathbf{j}}(\nabla_{\mathbf{x}}) G(\mathbf{C}, \mathbf{x}) = P_{\mathbf{j}}(\mathbf{C}, \mathbf{x}) G(\mathbf{C}, \mathbf{x}), \quad (\text{A6})$$

where P is a polynomial of order $\ell(\mathbf{j})$ in \mathbf{x} . Mathematical induction also shows, that P only contains monomials in \mathbf{x} of either even or odd order. The coefficients of P can be expressed in terms of the elements of \mathbf{C}^{-1} , but no attempt will be made here to give an explicit formula, because the expressions for any finite order polynomial can be derived iteratively. Up to order three the derivatives of G are given by (using summation convention)

$$\frac{\partial}{\partial x_j} G = \left[-C_{j\alpha}^{-1} x_{\alpha} \right] G \quad (\text{A7a})$$

$$\frac{\partial^2}{\partial x_j \partial x_k} G = \left[C_{j\alpha}^{-1} C_{k\beta}^{-1} x_{\alpha} x_{\beta} - C_{jk}^{-1} \right] G \quad (\text{A7b})$$

$$\begin{aligned} \frac{\partial^3}{\partial x_j \partial x_k \partial x_l} G &= \left[-C_{j\alpha}^{-1} C_{k\beta}^{-1} C_{l\gamma}^{-1} x_{\alpha} x_{\beta} x_{\gamma} \right. \\ &\quad \left. + (C_{jk}^{-1} C_{l\alpha}^{-1} + C_{jl}^{-1} C_{k\alpha}^{-1} \right. \\ &\quad \left. + C_{kl}^{-1} C_{j\alpha}^{-1}) x_{\alpha} \right] G. \end{aligned} \quad (\text{A7c})$$

Terms of the form $\mathcal{M}(\mathbf{x})G$ will be called monomial products of G in the following. Such products can be expressed in terms of derivatives of G . Applying a Fourier transform to Eq. (A6) and using of Eqs. (A3a), (A3b) and (A5) first gives

$$\mathcal{M}_{\mathbf{j}}(i\omega)G(\mathbf{C}^{-1}, \omega) = P_{\mathbf{j}}(\mathbf{C}, i\nabla_{\omega})G(\mathbf{C}^{-1}, \omega). \quad (\text{A8})$$

Substituting $i\omega$ by \mathbf{x} and \mathbf{C} by $-\mathbf{C}^{-1}$ (thus $\omega^t \mathbf{C} \omega$ by $\mathbf{x}^t \mathbf{C}^{-1} \mathbf{x}$) then finally yields

$$\mathcal{M}_{\mathbf{j}}(\mathbf{x})G(\mathbf{C}, \mathbf{x}) = P_{\mathbf{j}}(-\mathbf{C}^{-1}, -\nabla_{\mathbf{x}})G(\mathbf{C}, \mathbf{x}). \quad (\text{A9})$$

Up to order three the monomial products of G therefore read

$$x_j G = \left[-C_{j\alpha} \frac{\partial}{\partial x_{\alpha}} \right] G \quad (\text{A10a})$$

$$x_j x_k G = \left[C_{j\alpha} C_{k\beta} \frac{\partial^2}{\partial x_{\alpha} \partial x_{\beta}} + C_{jk} \right] G \quad (\text{A10b})$$

$$\begin{aligned} x_j x_k x_l G = & \left[-C_{j\alpha} C_{k\beta} C_{l\gamma} \frac{\partial^3}{\partial x_{\alpha} \partial x_{\beta} \partial x_{\gamma}} \right. \\ & - (C_{jk} C_{l\alpha} + C_{jl} C_{k\alpha} \\ & \left. + C_{kl} C_{j\alpha}) \frac{\partial}{\partial x_{\alpha}} \right] G. \end{aligned} \quad (\text{A10c})$$

4. Moments of Gauss functions

Integrating Eq. (A9) with respect to \mathbf{x} yields expressions for the moments of G . Because integrals of derivatives of G are vanishing, the moment is determined by the constant part of the polynomial $P_{\mathbf{j}}$. This coefficient will be non-zero only for even moments. The odd moments of G all evaluate to zero (as can also be seen from symmetry considerations). The first non-vanishing moments are given by

$$\int_{\mathbf{x}} G \, d\mathbf{x} = 1 \quad (\text{A11a})$$

$$\int_{\mathbf{x}} x_j x_k G \, d\mathbf{x} = C_{jk} \quad (\text{A11b})$$

$$\begin{aligned} \int_{\mathbf{x}} x_j x_k x_l x_m G \, d\mathbf{x} = & C_{jk} C_{lm} + C_{jl} C_{km} \\ & + C_{jm} C_{kl}. \end{aligned} \quad (\text{A11c})$$

5. Gauss functions in convolutions

Convolutions of the form $[\mathcal{M}_{\mathbf{j}}(\mathbf{x})G(\mathbf{C}, \mathbf{x})] * f(\mathbf{x})$ can be expressed in terms of derivatives of the convolution $G * f$. This can be derived straightforwardly by first expressing $\mathcal{M}(\mathbf{x})G$ by derivatives of G and then applying Eq. (A3d). One finds

$$[\mathcal{M}_{\mathbf{j}}(\mathbf{x})G(\mathbf{C}, \mathbf{x})] * f(\mathbf{x}) = P_{\mathbf{j}}(-\mathbf{C}^{-1}, -\nabla_{\mathbf{x}}) \times [G(\mathbf{C}, \mathbf{x}) * f(\mathbf{x})]. \quad (\text{A12})$$

It is also possible to express convolutions of the form $G(\mathbf{C}, \mathbf{x}) * [\mathcal{M}_{\mathbf{j}}(\mathbf{x})f(\mathbf{x})]$ by derivatives of monomial products of $G * f$. This can be derived in Fourier space. So let F denote the Fourier transform of the expression under consideration.

$$\begin{aligned} F &:= \mathcal{F} \left\{ G(\mathbf{C}, \mathbf{x}) * [\mathcal{M}_{\mathbf{j}}(\mathbf{x})f(\mathbf{x})] \right\} \\ &= \hat{G}(\mathbf{C}, \omega) \mathcal{M}_{\mathbf{j}}(i\nabla_{\omega}) \hat{f}(\omega) \end{aligned} \quad (\text{A13})$$

Using the identity

$$\frac{1}{\hat{G}(\mathbf{C}, \omega)} = \sqrt{(2\pi)^N |\det(\mathbf{C}^{-1})|} G(\mathbf{C}^{-1}, i\omega) \quad (\text{A14})$$

leads to

$$\begin{aligned} F &= \hat{G}(\mathbf{C}, \omega) \mathcal{M}_{\mathbf{j}}(i\nabla_{\omega}) \left[\frac{\hat{G}(\mathbf{C}, \omega)}{\hat{G}(\mathbf{C}, \omega)} \hat{f}(\omega) \right] \\ &= \hat{G}(\mathbf{C}, \omega) \sqrt{(2\pi)^N |\det(\mathbf{C}^{-1})|} \mathcal{M}_{\mathbf{j}}(i\nabla_{\omega}) \\ &\quad \times \left\{ G(\mathbf{C}^{-1}, i\omega) [\hat{G}(\mathbf{C}, \omega) \hat{f}(\omega)] \right\}. \end{aligned} \quad (\text{A15})$$

Now the product rule of differentiation is applied to the term in the curly brackets. Using index-vectors the product rule can be written as

$$\begin{aligned} \mathcal{M}_{\mathbf{j}}(\nabla)[f(\mathbf{x})g(\mathbf{x})] &= \sum_{(\mathbf{j}', \mathbf{j}'') \in \mathcal{P}(\mathbf{j})} [\mathcal{M}_{\mathbf{j}'}(\nabla)f(\mathbf{x})] \\ &\quad \times [\mathcal{M}_{\mathbf{j}''}(\nabla)g(\mathbf{x})]. \end{aligned} \quad (\text{A16})$$

Here $\mathcal{P}(\mathbf{j})$ denotes the set of all $2^{\ell(\mathbf{j})}$ pairs $(\mathbf{j}', \mathbf{j}'')$ that can be obtained by distributing the components of \mathbf{j} on two vectors \mathbf{j}' and \mathbf{j}'' . Applying the product rule yields

$$F = \hat{G}(\mathbf{C}, \omega) \sqrt{(2\pi)^N |\det(\mathbf{C}^{-1})|} \sum_{(\mathbf{j}', \mathbf{j}'') \in \mathcal{P}(\mathbf{j})} \left\{ \mathcal{M}_{\mathbf{j}'}(i\nabla_{\omega}) G(\mathbf{C}^{-1}, i\omega) \right\} \left\{ \mathcal{M}_{\mathbf{j}''}(i\nabla_{\omega}) [\hat{G}(\mathbf{C}, \omega) \hat{f}(\omega)] \right\}. \quad (\text{A17})$$

Temporarily substituting $\mathbf{z} = -i\omega$ in the first bracket and using $G(\bullet, -\mathbf{x}) = G(\bullet, \mathbf{x})$ gives

$$\mathcal{M}_{\mathbf{j}'}(i\nabla_{\omega}) G(\mathbf{C}^{-1}, i\omega) = \mathcal{M}_{\mathbf{j}'}(\nabla_{\mathbf{z}}) G(\mathbf{C}^{-1}, \mathbf{z}) = P_{\mathbf{j}'}(\mathbf{C}^{-1}, \mathbf{z}) G(\mathbf{C}^{-1}, \mathbf{z}) = P_{\mathbf{j}'}(\mathbf{C}^{-1}, -i\omega) G(\mathbf{C}^{-1}, i\omega). \quad (\text{A18})$$

Now $G(\mathbf{C}^{-1}, i\omega)$ can be written in front of the sum. Using Eq. (A14) some factors cancel out and it remains

$$F = \sum_{(\mathbf{j}', \mathbf{j}'') \in \mathcal{P}(\mathbf{j})} P_{\mathbf{j}'}(\mathbf{C}^{-1}, -i\omega) \mathcal{M}_{\mathbf{j}''}(i\nabla_\omega) [\hat{G}(\mathbf{C}, \omega) \hat{f}(\omega)]. \quad (\text{A19})$$

Switching back to real space finally gives the desired relation

$$G(\mathbf{C}, \mathbf{x}) * [\mathcal{M}_{\mathbf{j}}(\mathbf{x}) f(\mathbf{x})] = \sum_{(\mathbf{j}', \mathbf{j}'') \in \mathcal{P}(\mathbf{j})} P_{\mathbf{j}'}(\mathbf{C}^{-1}, -\nabla_x) \left\{ \mathcal{M}_{\mathbf{j}''}(\mathbf{x}) [G(\mathbf{C}, \mathbf{x}) * f(\mathbf{x})] \right\}. \quad (\text{A20})$$

Appendix B: Conditioned moments $\mathbf{m}^{(k)}$

The somewhat lengthy calculations leading to Eq. (17) are given below. The function argument of $\mathbf{M}(\tau)$ and $\mathbf{C}(\tau)$ will be omitted for notational simplicity. Partial derivation with respect to x_i will be denoted by ∂_i and Einsteins summation convention will be used. Starting with Eq. (16), inserting Eqs. (13b) and (15) and interchanging the order of integration gives

$$m^{*(0)}(\mathbf{x}) = \int_{\mathbf{z}} G(\mathbf{V}, \mathbf{x} - \mathbf{z}) \int_{\mathbf{z}'} \rho(\mathbf{z}, \mathbf{z}', \tau) \int_{\mathbf{x}'} G(\mathbf{C}, \mathbf{x}' - \mathbf{z}' - \mathbf{M} \cdot (\mathbf{x} - \mathbf{z})) d\mathbf{x}' d\mathbf{z}' d\mathbf{z} \quad (\text{B1a})$$

$$m_i^{*(1)}(\mathbf{x}, \tau) = \int_{\mathbf{z}} G(\mathbf{V}, \mathbf{x} - \mathbf{z}) \int_{\mathbf{z}'} \rho(\mathbf{z}, \mathbf{z}', \tau) \int_{\mathbf{x}'} (x'_i - x_i) G(\mathbf{C}, \mathbf{x}' - \mathbf{z}' - \mathbf{M} \cdot (\mathbf{x} - \mathbf{z})) d\mathbf{x}' d\mathbf{z}' d\mathbf{z} \quad (\text{B1b})$$

$$m_{ij}^{*(2)}(\mathbf{x}, \tau) = \int_{\mathbf{z}} G(\mathbf{V}, \mathbf{x} - \mathbf{z}) \int_{\mathbf{z}'} \rho(\mathbf{z}, \mathbf{z}', \tau) \int_{\mathbf{x}'} (x'_i - x_i)(x'_j - x_j) G(\mathbf{C}, \mathbf{x}' - \mathbf{z}' - \mathbf{M} \cdot (\mathbf{x} - \mathbf{z})) d\mathbf{x}' d\mathbf{z}' d\mathbf{z} \quad (\text{B1c})$$

The integrals with respect to \mathbf{x}' can be expressed in terms of the moments of the involved Gauss function (see Sec. (A 4)). Using the definition of $m^{(0)}$ then allows to express $m^{*(0)}$ by a convolution.

$$m^{*(0)}(\mathbf{x}) = G(\mathbf{V}, \mathbf{x}) * m^{(0)}(\mathbf{x}) \quad (\text{B2})$$

$$(\text{B3})$$

The other moments so far read

$$m_i^{*(1)}(\mathbf{x}, \tau) = \int_{\mathbf{z}} G(\mathbf{V}, \mathbf{x} - \mathbf{z}) \int_{\mathbf{z}'} \rho(\mathbf{z}, \mathbf{z}', \tau) [z'_i - x_i + M_{ii'}(x_{i'} - z_{i'})] d\mathbf{z}' d\mathbf{z} \quad (\text{B4a})$$

$$m_{ij}^{*(2)}(\mathbf{x}, \tau) = \int_{\mathbf{z}} G(\mathbf{V}, \mathbf{x} - \mathbf{z}) \int_{\mathbf{z}'} \rho(\mathbf{z}, \mathbf{z}', \tau) [C_{ij} + (z'_i - x_i + M_{ii'}(x_{i'} - z_{i'})) \times (z'_j - x_j + M_{jj'}(x_{j'} - z_{j'}))] d\mathbf{z}' d\mathbf{z}. \quad (\text{B4b})$$

Sorting the terms in rectangular brackets by powers of the components of $\mathbf{z}' - \mathbf{z}$ and using the definitions of the moments $\mathbf{m}^{(k)}$, allows the integrals with respect to \mathbf{z}' to be expressed by the moments $\mathbf{m}^{(k)}$.

$$m_i^{*(1)}(\mathbf{x}, \tau) = \int_{\mathbf{z}} G(\mathbf{V}, \mathbf{x} - \mathbf{z}) \left[m_i^{(1)}(\mathbf{z}, \tau) - (\delta_{ii'} - M_{ii'})(x_{i'} - z_{i'}) m^{(0)}(\mathbf{z}) \right] d\mathbf{z} \quad (\text{B5a})$$

$$m_{ij}^{*(2)}(\mathbf{x}, \tau) = \int_{\mathbf{z}} G(\mathbf{V}, \mathbf{x} - \mathbf{z}) \left[m_{ij}^{(2)}(\mathbf{z}, \tau) + C_{ij} m^{(0)}(\mathbf{z}) - (\delta_{jj'} - M_{jj'})(x_{j'} - z_{j'}) m_i^{(1)}(\mathbf{z}, \tau) - (\delta_{ii'} - M_{ii'})(x_{i'} - z_{i'}) m_j^{(1)}(\mathbf{z}, \tau) + (\delta_{ii'} - M_{ii'})(x_{i'} - z_{i'}) (\delta_{jj'} - M_{jj'})(x_{j'} - z_{j'}) m^{(0)}(\mathbf{z}) \right] d\mathbf{z}. \quad (\text{B5b})$$

Now the relation $\int_{\mathbf{z}} (x_i - z_i) f(\mathbf{x} - \mathbf{z}) g(\mathbf{z}) d\mathbf{z} = [x_i f(\mathbf{x})] * g(\mathbf{x})$ can be used to express the noisy moments as convolutions. Function arguments can now be omitted without confusion (G refers to $G(\mathbf{V}, \mathbf{x})$).

$$m_i^{*(1)} = G * m_i^{(1)} - (\delta_{ii'} - M_{ii'}) [x_{i'} G] * m^{(0)} \quad (\text{B6a})$$

$$m_{ij}^{*(2)} = G * m_{ij}^{(2)} + C_{ij} G * m^{(0)} - (\delta_{ii'} - M_{ii'}) [x_{i'} G] * m_j^{(1)} - (\delta_{jj'} - M_{jj'}) [x_{j'} G] * m_i^{(1)}$$

$$+(\delta_{ii'} - M_{ii'})(\delta_{jj'} - M_{jj'})[x_{i'}x_{j'}G] * m^{(0)}. \quad (\text{B6b})$$

Because G is a Gauss function, the monomial products $x_i G$ and $x_i x_j G$ can be expressed by derivatives. Inserting the definition of \mathbf{C} (Eq. (14)) and resorting terms subsequently leads to

$$m_i^{*(1)} = G * m_i^{(1)} + (\delta_{ii'} - M_{ii'})V_{i'k}[\partial_k G] * m^{(0)} \quad (\text{B7a})$$

$$m_{ij}^{*(2)} = G * m_{ij}^{(2)} + \{(\delta_{jj'} - M_{jj'})V_{ij'} + (\delta_{ii'} - M_{ii'})V_{i'j}\}G * m^{(0)} + (\delta_{ii'} - M_{ii'})V_{i'k}[\partial_k G] * m_j^{(1)} \\ + (\delta_{jj'} - M_{jj'})V_{j'k}[\partial_k G] * m_i^{(1)} + (\delta_{ii'} - M_{ii'})V_{i'k}(\delta_{jj'} - M_{jj'})V_{j'l}[\partial_k \partial_l G] * m^{(0)}. \quad (\text{B7b})$$

Introducing the abbreviation $\mathbf{Q} := (\mathbf{Id} - \mathbf{M})\mathbf{V}$ and using the relation $(\partial f) * g = \partial(f * g)$ this can be written as

$$m_i^{*(1)} = G * m_i^{(1)} + Q_{ii'}\partial_{i'}(G * m^{(0)}) \quad (\text{B8a})$$

$$m_{ij}^{*(2)} = G * m_{ij}^{(2)} + (Q_{ij} + Q_{ji})G * m^{(0)} + Q_{ii'}\partial_{i'}(G * m_j^{(1)}) + Q_{jj'}\partial_{j'}(G * m_i^{(1)}) \\ + Q_{ii'}Q_{jj'}\partial_{i'}\partial_{j'}(G * m^{(0)}). \quad (\text{B8b})$$

Substituting $G * m^{(0)} = m^{*(0)}$ according to Eq. (B2) gives

$$m_i^{*(1)} = G * m_i^{(1)} + Q_{ii'}\partial_{i'}m^{*(0)} \quad (\text{B9a})$$

$$m_{ij}^{*(2)} = G * m_{ij}^{(2)} + (Q_{ij} + Q_{ji})m^{*(0)} + Q_{ii'}\partial_{i'}(G * m_j^{(1)}) + Q_{jj'}\partial_{j'}(G * m_i^{(1)}) + Q_{ii'}Q_{jj'}\partial_{i'}\partial_{j'}m^{*(0)}. \quad (\text{B9b})$$

Now $G * m_i^{(1)} = m_i^{*(1)} - Q_{ii'}\partial_{i'}m^{*(0)}$ can be substituted, what leads to

$$m_{ij}^{*(2)} = G * m_{ij}^{(2)} + (Q_{ij} + Q_{ji} - Q_{ii'}Q_{jj'}\partial_{i'}\partial_{j'})m^{*(0)} + Q_{ii'}\partial_{i'}m_j^{*(1)} + Q_{jj'}\partial_{j'}m_i^{*(1)}. \quad (\text{B10})$$

Putting these results together and using Eq. (4) to express $\mathbf{m}^{(k)}$ in terms of $\mathbf{h}^{(k)}$ and $m^{(0)}$ yields the final expressions for the noisy moments $\mathbf{m}^{(k)}$.

$$m^{*(0)} = G * m^{(0)} \quad (\text{B11a})$$

$$m_i^{*(1)} = G * (h_i^{(1)}m^{(0)}) + Q_{ii'}\partial_{i'}m^{*(0)} \quad (\text{B11b})$$

$$m_{ij}^{*(2)} = G * (h_{ij}^{(2)}m^{(0)}) + (Q_{ij} + Q_{ji} - Q_{ii'}Q_{jj'}\partial_{i'}\partial_{j'})m^{*(0)} + Q_{ii'}\partial_{i'}m_j^{*(1)} + Q_{jj'}\partial_{j'}m_i^{*(1)} \quad (\text{B11c})$$

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